Quantum Graphs which Optimize the Spectral Gap

Ram Band

Technion - Israel Institute of Technology

Joint work with Guillaume Lévy, Université Pierre et Marie Curie, Paris
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Eigenvalue optimization problems (for domains)

Fixing the topology, total volume and boundary conditions,
we seek for the shape which maximizes\minimizes an eigenvalue.

Simply connected domains

Faber-Krahn [Dirichlet conditions]: the ball minimizes λ_1 *(no sense maximizing).*

Krahn-Szegö [Dirichlet conditions]: No minimizer for λ_2,
but union of two balls serves as an *infimizer*.

Szegö-Weinberger [Neumann conditions]: the ball maximizes λ_1 *(no sense minimizing).*

Multi connected domains

Payne-Weinberger: Planar domains with a single hole,
Dirichlet on outer boundary and Neumann on inner.
Fixing total area and length of outer boundary - annulus (concentric circles) maximizes λ_1.

More works by: Ashbaugh-Chatelain, Ashbaugh-Benguria, Exner-Mantile, Flucher,
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Outline

From a Discrete graph to a Quantum graph

$\mathcal{G}$ a discrete graph with $E < \infty$ edges and $V < \infty$ vertices. Space of edge lengths:

$\mathscr{L}_{\mathcal{G}} := \left\{ (l_1, \ldots, l_E) \in \mathbb{R}^E \;\middle|\; \sum_{e=1}^{E} l_e = 1 \text{ and } \forall e,\ l_e > 0 \right\}$

$\Gamma(\mathcal{G};\ \underline{l})$ denotes the metric graph obtained from $\mathcal{G}$ with edge lengths $\underline{l} \in \mathscr{L}_{\mathcal{G}}$.

Namely, the e^{th} edge corresponds to an interval $[0, l_e]$

Consider the following eigenvalue equation on each $[0, l_e]$: $\quad -\frac{\mathrm{d}^2}{\mathrm{d}x_e^2} f\Big|_e = k^2 f\Big|_e$,

with the Neumann (Kirchhoff) vertex conditions:

$$\text{Continuity} \qquad \forall e_1, e_2 \sim v\,;\ \ f\big|_{e_1}(v) = f\big|_{e_2}(v)$$

$$\text{Vanishing sum of derivatives} \qquad \sum_{e \sim v} \frac{\mathrm{d}}{\mathrm{d}x_e} f\bigg|_e (v) = 0$$

The spectrum, $\left\{k_n^2\right\}_{n=1}^{\infty}$ is discrete and bounded from below:

$$0 = k_0 < k_1 \le k_2 \le \ldots$$

We call k_1 the spectral gap of the graph.

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Spectral gap dependence on edge lengths

$\mathscr{L}_{\mathcal{G}} := \left\{ (l_1, \ldots, l_E) \in \mathbb{R}^E \,\middle|\, \sum_{e=1}^{E} l_e = 1 \text{ and } \forall e,\ l_e > 0 \right\}.$

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Spectral gap is denoted $k_1[\Gamma(\mathcal{G};\ \underline{l})]$. Note: $k_1[\Gamma(\mathcal{G};\ \underline{l})]$ is continuous in $\underline{l}$,
which leads to consider also $\underline{l} \in \partial\mathscr{L}_{\mathcal{G}}$ (some edge lengths vanish),
possibly changing the topology of $\Gamma(\mathcal{G};\ \underline{l})$.

Definition 1.

- $\Gamma(\mathcal{G};\ \underline{l}^*)$ a maximizer of $\mathcal{G}$ if $\underline{l}^* \in \mathscr{L}_{\mathcal{G}}$ and $k_1[\Gamma(\mathcal{G};\ \underline{l}^*)] \geq k_1[\Gamma(\mathcal{G};\ \underline{l})]$, $\forall \underline{l} \in \mathscr{L}_{\mathcal{G}}$.
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- Same definitions for minimizer and infimizer.

- Supremizer and infimizer always exist.
  What about maximizer\minimizer?
- Which graphs are spectral gap optimizers?

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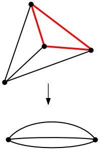

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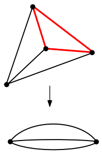

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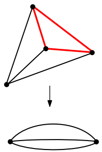

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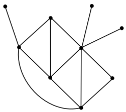

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Quantum Graphs which Optimize the Spectral Gap

- Supremizer and infimizer always exist. What about maximizer\minimizer?
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A few examples

Star graph with $E \geq 2$ edges

Infimum (no minimum): $k_1(1,0,\ldots 0) = \pi$,
Maximum: $k_1(1/E,\ldots,1/E) = \frac{E}{2}\pi$ (equilateral star)
(Recall: total edge length $= 1$)

Flower graph with $E \geq 2$ edges

Infimum (no minimum): $k_1(1,0,\ldots 0) = 2\pi$,
Maximum: $k_1(1/E,\ldots,1/E) = E\pi$ (equilateral flower)
[Kennedy, Kurasov, Malenová, Mugnolo '16]

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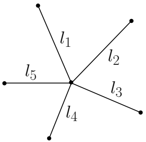

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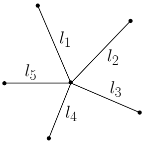

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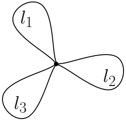

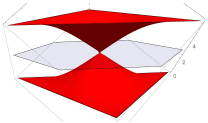

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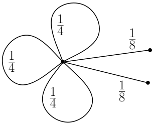

Stower (Flétoile) graph with E_p petals, E_l leaves

Infimum (no minimum): $k_1(0\ldots,0,1) = \pi$,

Maximum: $k_1(\underline{l}) = (E_p + \frac{E_l}{2})\pi$,

where $\underline{l} = \frac{1}{2E_p+E_l}(\underbrace{2,\ldots,2}_{E_p},\underbrace{1,\ldots,1}_{E_l})$ ("equilateral" stower),

assuming $E_p + E_l \geq 2$ and $(E_p, E_l) \notin (1,1)$. [Shown in future slide].

This generales stars and flowers results.

Quantum Graphs which Optimize the Spectral Gap

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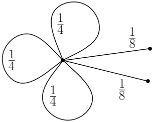

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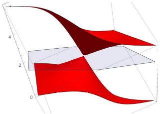

$E_p = 2$

$E_l = 1$

Infimum: $k_1(0,0,1) = \pi$,

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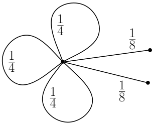

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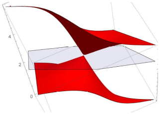

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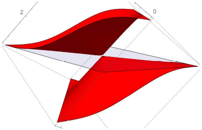

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Continuous family of infima: $k_1(0,t,1-t) = \pi$,

Continuous family of maxima: $k_1(1-2t,t,t) = 2\pi$

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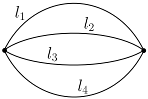

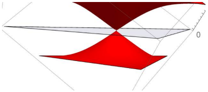

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Mandarin graph with E edges

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Length dependence figures - courtesy of Lior Alon

- Which graphs have not only supremizer\infimizer, but also maximizer\minimizer?
- Which graphs are spectral gap optimizers?

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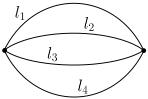

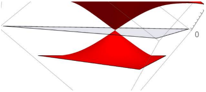

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Mandarin graph with E edges

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Maximum: $k_1(1/E, \ldots, 1/E) = E\pi$.

[Kennedy, Kurasov, Malenová, Mugnolo '16]

Length dependence figures - courtesy of Lior Alon

- Which graphs have not only supremizer\infimizer, but also maximizer\minimizer?
- Which graphs are spectral gap optimizers?

Lower bounds - Known results

$$k_1[\Gamma] \geq \pi$$

with equality iff Γ is a single edge [Nicaise '87; Friedlander '05; Kurasov, Naboko '14].

If Γ has all vertex degrees even then

$$k_1[\Gamma] \geq 2\pi, \qquad \text{[Kurasov, Naboko '14]}$$

with a single loop achieving equality (for example).

Remaining questions:

- What about other topologies?
- What are all possible minimizers\infimizers?

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Infimizers - Solution

A **bridge** is an edge whose removal dissconnects the graph.

Theorem 2 (Band, Lévy).

1. *Let $\mathcal{G}$ be a graph with a bridge. Then*
   1.1 *The infimal spectral gap of $\mathcal{G}$ equals π.*
   1.2 *The unique infimizer is the unit interval.*
2. *Let $\mathcal{G}$ be a bridgeless graph. Then*
   2.1 *The infimal spectral gap of $\mathcal{G}$ equals 2π.*
   2.2 *Any infimizer is a symmetric necklace graph.*

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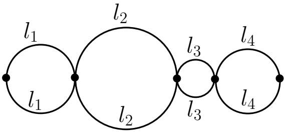

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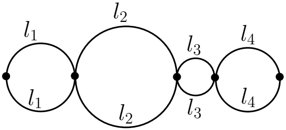

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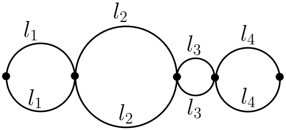
- When is there a minimum?
- Proof idea - rearrangment method on graphs.



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Upper bounds - Known results

- Global bound

$$k_1[\Gamma] \leq E\pi,$$

equality if and only if Γ is an equilateral mandarin or equilateral flower [Kennedy, Kurasov, Malenová, Mugnolo '16].

This fully answers optimization for flowers and mandarins:
supremizers (also maximizers) are equilateral.

- If Γ is a tree then

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equality if and only if Γ is an equilateral star [Rohleder '16].

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Upper bounds - Further progress

Proposition 3 (Band, Lévy).

If Γ is a tree with E_l leaves then $k_1[\Gamma] \leq \frac{E_l}{2}\pi$.

Proof idea.

$d(\Gamma) := \max\{d(x,y) \big| x,y \in \Gamma\}$ graph diameter.

Combine $k_1[\Gamma] \leq \frac{\pi}{d(\Gamma)}$ with $d(\Gamma) \geq \frac{2}{E_l}$ (the latter true for trees).

$\square$

Proposition 4 (Band, Lévy).

Let $\mathcal{G}$ be a graph with E edges, out of which E_l are leaves.
If $(E, E_l) \notin \{(1,1),(1,0),(2,1)\}$ then $\forall\ \underline{l} \in \mathscr{L}_{\mathcal{G}}, \quad k_1[\Gamma(\mathcal{G};\ \underline{l})] \leq \pi\left(E - \frac{E_l}{2}\right)$.
Assuming $(E, E_l) \notin \{(2,0),(3,2)\}$ equality above implies $\Gamma(\mathcal{G};\ \underline{l})$ is either an equilateral mandarin $(E_l = 0)$ or an equilateral stower $(E_l \geq 0)$.

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Proof idea.

Take Γ and attach two vertices to obtain Γ' (illegal move in our game). Get $k_1(\Gamma) \le k_1(\Gamma')$.

Repeatedly attach all inner vertices to obtain a stower with E_l leaves and $E - E_l$ petals.

Use bound on stowers: $k_1[\Gamma] \le \pi\left(E - \frac{E_l}{2}\right)$ [to appear in a future slide] $\square$

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Spectral gap as a simple eigenvalue - Critical points

Try to find supremizers by seeking for local critical points in $\mathscr{L}_{\mathcal{G}}$.

Derivatives with respect to edge lengths may be calculated for simple eigenvalues.

Theorem 5 (Band, Lévy).

Let $\mathcal{G}$ be a discrete graph and $\underline{l} \in \mathscr{L}_{\mathcal{G}}$.

Assume that $\Gamma(\mathcal{G};\ \underline{l})$ is a supremizer of $\mathcal{G}$ with simple spectral gap $k_1[\Gamma(\mathcal{G};\ \underline{l})]$.

Then $\Gamma(\mathcal{G};\ \underline{l})$ is not a unique supremizer:

there exists $\underline{l}^* \in \overline{\mathscr{L}_{\mathcal{G}}}$ s.t. $\Gamma(\mathcal{G};\ \underline{l}^*)$ is an equilateral mandarin and

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Proof ingredients.

- A supremizer is a critical point of some $\mathscr{L}_{\hat{\mathcal{G}}}$ ($\hat{\mathcal{G}}$ maybe different than $\mathcal{G}$).
- $\forall e \quad \frac{\partial}{\partial l_e}\left(k^2\right) = -\left(f'^2 + k^2 f^2\right)\Big|_e$ where f eigenfunction which corresponds to k.
- This implies restrictions on eigenfunction derivatives.
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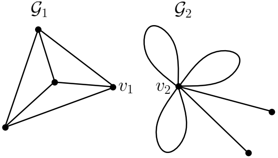
Gluing graphs - Vertex connectivity one

Let $\mathcal{G}_1, \mathcal{G}_2$ be discrete graphs, and v_i $(i = 1, 2)$ be a vertex of $\mathcal{G}_i$.
Let $\mathcal{G}$ be the graph obtained by identifying (gluing) v_1 and v_2.
If we know the supremizers Γ_1, Γ_2 of $\mathcal{G}_1$, $\mathcal{G}_2$,

can we tell the supremizer of $\mathcal{G}$?



Corollary 6.

Let $\mathcal{G}_1, \mathcal{G}_2$ be discrete graphs.
Let $\mathcal{G}$ obtained by identifying two non-leaf vertices v_1 and v_2.

If the (unique) supremizer of $\mathcal{G}_i$ is the "equilateral" stower with $E_p^{(i)}$ petals and $E_l^{(i)}$ leaves, such that $E_p^{(i)} + E_l^{(i)} \geq 2$, then the (unique) supremizer of $\mathcal{G}$ is an "equilateral" stower with $E_p^{(1)} + E_p^{(2)}$ petals and $E_l^{(1)} + E_l^{(2)}$ leaves.

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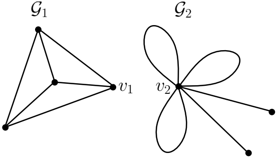

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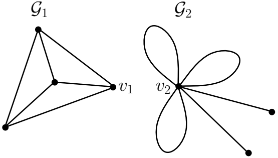

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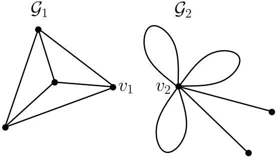

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Corollary 7.

Let $\mathcal{G}$ be a stower with $E_p + E_l \geq 2$ and $(E_p, E_l) \neq (1,1)$. Then a maximizer is the "equilateral" stower graph with spectral gap $\pi\left(E_p + \frac{E_l}{2}\right)$.
This maximizer is unique for $\left(E_p, E_l\right) \notin \{(2,0),(1,2)\}$.

Proof idea.

Prove the statement for "small" stowers. Then glue them to construct any stower. □

Recall

Proposition 4:

Let $\mathcal{G}$ be a graph with E edges, out of which E_l are leaves.
If $(E, E_l) \notin \{(1,1),(1,0),(2,1)\}$ then $\forall\ \underline{l} \in \mathscr{L}_{\mathcal{G}}, \quad k_1\left[\Gamma\left(\mathcal{G};\ \underline{l}\right)\right] \leq \pi\left(E - \frac{E_l}{2}\right)$.
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Summary

- Optimization problem fully solved for infimizers\minimizers.
- Supremizers
  - Improved upper bounds by conditioning on number of leaves, $k_1 \leq \pi\left(E - \frac{E_l}{2}\right)$ (global) and $k_1 \leq \pi\frac{E_l}{2}$ (for trees).
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Supremizer candidates are stowers and mandarins (are there any others?)

$\Rightarrow$ lower bounds on supremal spectral gap

Getting to a stower gives $\pi\left(\beta + \frac{E_l}{2}\right)$,
where $\beta := E - V + 1$ is the graph's first Betti number.

Getting to a mandarin:

Partition vertices $V = V_1 \cup V_2$.

$E(V_1, V_2) :=$ # of edges connecting V_1 to V_2.

Maximal spectral gap *among all mandarins is*
$\pi \cdot \max_{V_1, V_2} E(V_1, V_2)$. (Cheeger-like constant)

Compare $\pi\left(\beta + \frac{E_l}{2}\right)$ (stower) with $\pi \cdot \max_{V_1, V_2} E(V_1, V_2)$ (mandarin).

$E(V_1, V_2) = \beta + 1 - (\beta_1 + \beta_2)$, where β_i is the Betti number of V_i graph.

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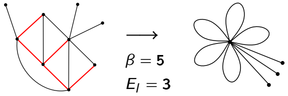

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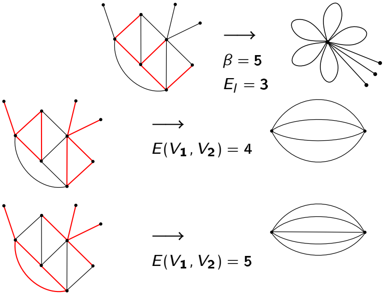
where $\beta := E - V + 1$ is the graph's first Betti number.

Getting to a mandarin:

Partition vertices $V = V_1 \cup V_2$.

$E(V_1, V_2) :=$ # of edges connecting V_1 to V_2.

Maximal spectral gap *among all mandarins is*
$\pi \cdot \max_{V_1,V_2} E(V_1, V_2)$. (Cheeger-like constant)



Compare $\pi\left(\beta + \frac{E_l}{2}\right)$ (stower) with $\pi \cdot \max_{V_1,V_2} E(V_1, V_2)$ (mandarin).

$E(V_1, V_2) = \beta + 1 - (\beta_1 + \beta_2)$, where β_i is the Betti number of V_i graph.

If $E_l \leq 1$ then mandarin wins if and only if we find $\beta_1 = \beta_2 = 0$.

If $E_l \geq 2$ then mandarin never wins (possibility for a tie).

Summary

Supremizer candidates are stowers and mandarins (are there any others?)

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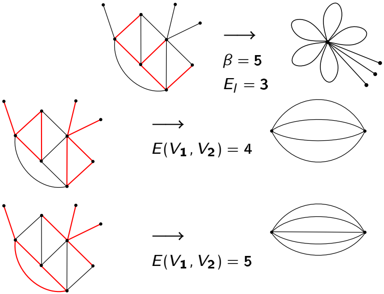

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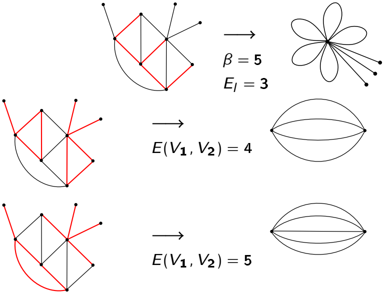

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Leads to conjectures....

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Quantum Graphs which Optimize the Spectral Gap

Ram Band

Technion - Israel Institute of Technology

Joint work with Guillaume Lévy, Université Pierre et Marie Curie, Paris
(arXiv:1608.00520)

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